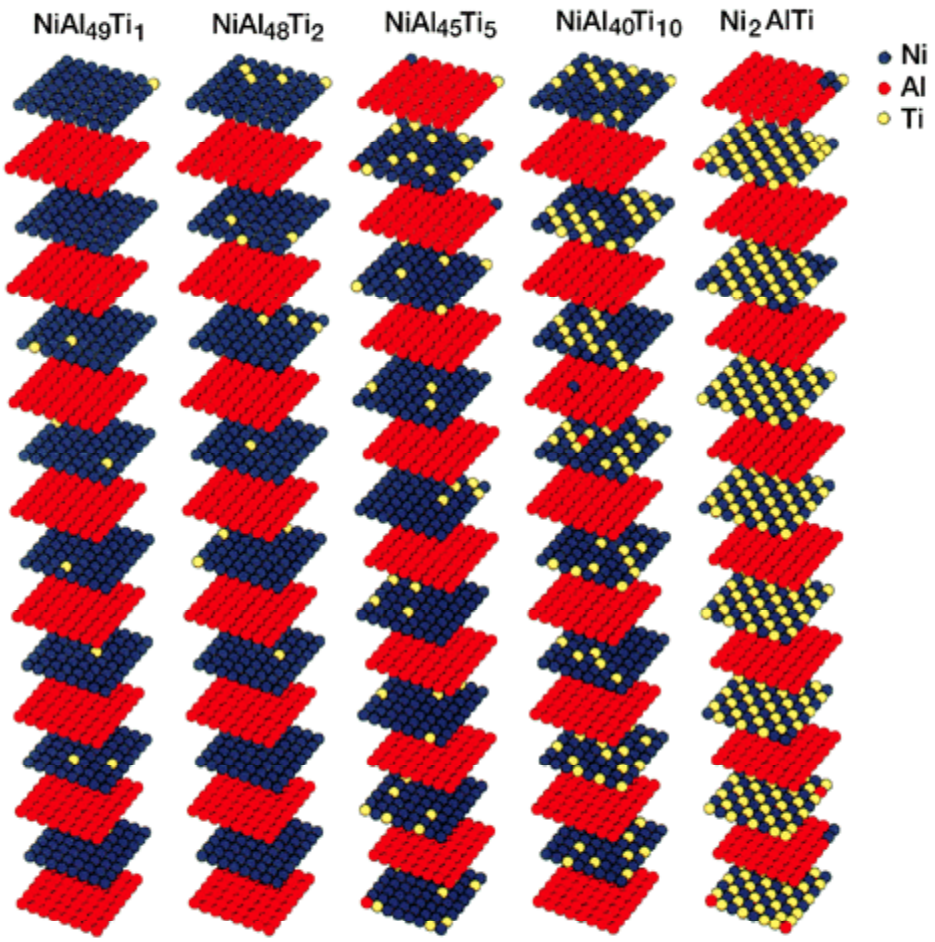
BFS Method for Alloys Optimized and Verified for the Study of Ordered Intermetallic Material

The aerospace industry has a need for new metallic alloys that are lightweight and have high strength at elevated temperatures. However, the current design method for new materials is largely experimental, requiring substantial capital investment in processing the material and in determining the material's microstructure and properties. Theoretical methods that would narrow the field of promising candidate materials could substantially reduce cost and development time.

The BFS (Bozzolo, Ferrante, and Smith) method is a new, computationally efficient and physically sound quantum semi-perturbative approach for describing metals and their defects. Based on a simple interpretation of the alloy formation process that identifies strain and chemical contributions to the energy of the alloy, the method provides an atom-by-atom description of an alloy. Its implementation requires little more than algebra and the solution of transcendental equations.

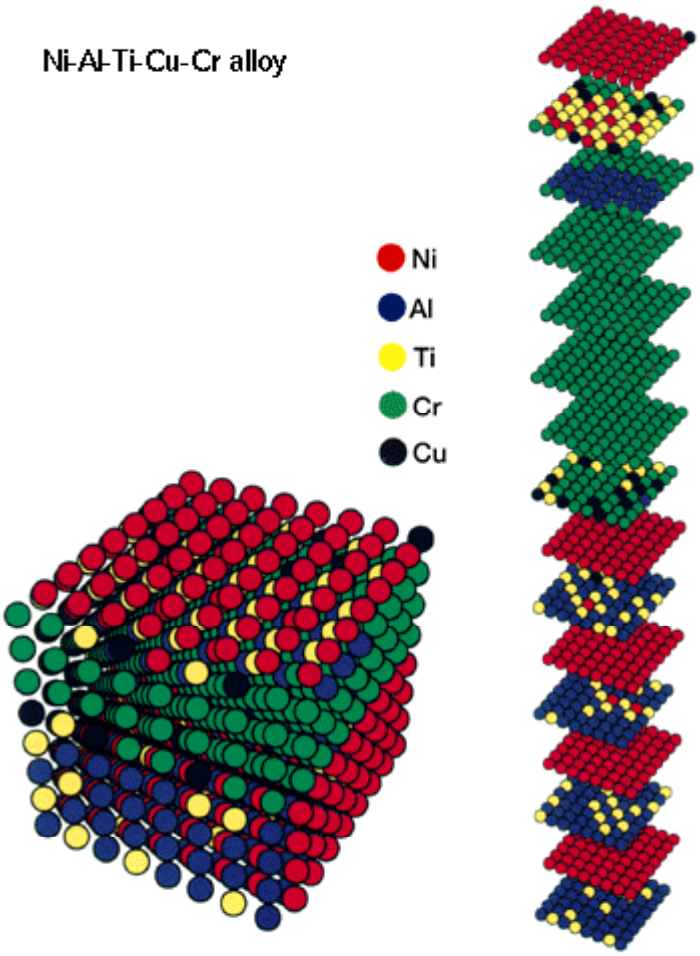
In contrast, methods previous to BFS suffered from many limitations. The state-of-the-art nonatomistic approaches rely heavily on developing a substantial data base, then extrapolating to predict new properties. Although this approach has been successful, it leads to incremental rather than revolutionary improvements. Other approaches--such as first-principles, quantum mechanical methods, and other competing semi-empirical methods--suffer from more serious limitations. Quantum mechanical methods, although in principle the best, require so much CPU time as to make calculations on applied problems infeasible. Competing semi-empirical methods are limited to a few face-centered-cubic metals and are not successful in predicting most alloy properties.

At the NASA Lewis Research Center, we have demonstrated (ref. 1) that BFS can investigate the properties of a large number of alloys with a minimum computational effort on low-level computers. This screening allows the selection of the best alloy candidates for a particular application and, therefore, promises large cost savings over current approaches.



Ni-Al-Ti alloys modeled with BFS, for different Ti concentrations. Above 5 at.% Ti, the formation of Heusler precipitates is seen. For 25 at.% Ti, the computational cell (1024 atoms) displays Heusler ordering with a few antistructural atoms.

BFS has been tested in a variety of situations, consistently giving results in excellent agreement with experimental results. More recently, the method has been optimized for modeling ordered intermetallic alloys that are of interest in aeronautical applications, including the determination of the defect structure of FeAl alloys (ref. 2) and the characterization of ternary and quaternary Ni_3Al-based alloys (ref. 3). Much of the recent effort, however, has focused on alloy design of NiAl-based materials. The complexity of the systems modeled range from three-component, two-phase alloys (such as the Ni-Al-Ti alloys shown in the first figure) to five-component, three-phase alloys that exhibit solute enrichment at the interfaces (as shown in the following figure). Such complex structures cannot be modeled by alternative techniques, and the accuracy of the predictions has been verified by appropriate experimental studies.



Ni-Al-Ti-Cu-Cr alloy modeled with BFS. The computational cell displays the formation of a Cr precipitate within the NiAl matrix. Also, the formation of the Heusler (Ni_2AlTi) phase is observed. Cu atoms are found only in the interface between NiAl and the a*-Cr precipitate.*

The BFS method is not limited solely to high-temperature structural alloy design. It can be applied to the design of high-performance alloys for any application. In addition to the design function, it can be used in place of or in conjunction with experiments to analyze the poorly understood mechanical and thermal properties of existing alloys. The method also has shown potential to perform revolutionary analysis of alloy structures and thin films and to be applied in interface-related studies (ref. 4).

References

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3. Bozzolo, G.; Ferrante, J.J.: Computer-Aided Mater. Design, vol. 2, 1995, p. 113.

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